

Comment on "Universally Diverging Gruneisen Parameter and the Magnetocaloric Effect Close to a Quantum Critical Point".

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In a recent Letter Zhu et al. [1] obtained scaling relations for the Gruneisen parameter $\Gamma \propto \beta/C$, where β is the thermal expansion and C the specific heat, of a heavy fermion system at the quantum critical point (QCP). We show here that generally this quantity yields information on the *shift* exponent governing the critical line of finite temperature transitions and not on the crossover exponent νz as obtained in Ref. [1]. We start with the Ehrenfest equation [2] relating the pressure derivative of the line of critical temperatures, T_N , to these thermodynamic quantities,

$$\frac{dT_N}{dP} = VT\frac{\Delta\beta}{\Delta C} = V\frac{\Delta\beta}{\Delta C/T} \quad (1)$$

where $\Delta\beta$ and ΔC are the *differences in thermal expansion and specific heat in the two phases* (the critical part), respectively. The thermal expansion is defined by

$$\beta = \frac{1}{V}\frac{\partial V}{\partial T} = -\kappa_T \frac{\partial^2 F}{\partial T \partial V}|_N. \quad (2)$$

The isothermal compressibility $\kappa_T = -(1/V)(\partial V/\partial P)$ is non-singular at the QCP. The volume thermal expansion, $\beta = 2\alpha_a + \alpha_c$ where α_i are the linear thermal expansion coefficients along different axes i . The critical line of finite temperature phase transitions close to the QCP is given by,

$$T_N \propto \frac{1}{u}|V - V_c|^\psi \propto \frac{1}{u}|P - P_c|^\psi \quad (3)$$

which defines the shift exponent ψ [3]. The critical temperature is reduced changing the volume by applying pressure in the system. The quantities V_c and P_c are the critical volume and pressure, respectively. From the equation above we obtain,

$$\frac{dT_N}{dP} \propto \frac{1}{u}|P - P_c|^{\psi-1} \propto T_N^{1-\frac{1}{\psi}}, \quad (4)$$

such that,

$$\lim_{T_N \rightarrow 0} V \frac{\Delta\beta}{\Delta C/T} = T_N^{1-\frac{1}{\psi}} \quad (5)$$

This is independent of any scaling ansatz relying only on the shape of the critical line and the Ehrenfest equation.

This result is inconsistent with that obtained by Zhu et al. [1] for $V = V_c$ and $d + z > 4$,

$$\frac{\Delta\beta}{\Delta C/T} \propto T^{1-\frac{1}{\nu z}}. \quad (6)$$

The reason for the discrepancy between Ehrenfest relation's result and the equation above, where ψ is replaced by νz , is that the purely Gaussian part of the quantum free energy which yields the results of Zhu et al. [1] ignores the critical Néel line. In the spin density wave theory, for $d + z \geq 4$, this line appears due to the dangerous irrelevant quartic interaction u , as in Eqs. 3, with $\psi = z/(d + z - 2)$ [4]. The purely Gaussian quantum free energy with $u = 0$ is unaware of the transition at T_N . These Gaussian quantum fluctuations must then be seen as *regular* contributions with respect to the *thermal phase transition* not contributing to the critical part of the physical quantities appearing in Eq. 1. Our results are obtained approaching the QCP from the magnetic side, i.e., with $T_N \rightarrow 0$. The quantum critical point is of course a special point of the critical line $T_N(P)$. They are particularly relevant for systems where T_N is vanishingly small but finite.

The results above are specially important since the temperature dependence of Eq. 5 becomes more singular than that of Ref. [1], Eq. 6, with ψ replaced by νz . In the spin density wave theory, this occurs exactly for $d + z > 4$, i.e., above the upper critical dimension, $d_c = 4$, which is the condition for breakdown of hyperscaling. In this case, the hyperscaling relation $\psi = \nu z$, which identifies the shift with the crossover exponent, breaks down for $d + z > 4$ due to the dangerous irrelevant quartic interaction u [4].

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